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Chemistry and Life Sciences

The Directorate of Chemistry and Life Sciences is responsible for research activities in chemistry and life sciences. A wide range of fundamental chemistry, biology, and behavioral research is supported to provide the Air Force with novel options to increase performance and operational flexibility. The chemistry effort in the directorate supports the structural materials activities in the Directorate of Aerospace and Materials Sciences to make an integrated AFOSR structural materials program. Although the program descriptions that follow are specific subareas of interest, there is interest in exploring novel ideas that bridge the disciplines. The interfaces between biology and chemistry, biology and physics, psychology and physics, or biology and behavior often provide the insights necessary for technological advances. Creativity is encouraged in suggesting novel scientific Approaches for our consideration.

Polymer Chemistry

The goal of this research area is to gain a better understanding of the influence of chemical structures and processing conditions on the properties and behaviors of polymeric and organic materials. This understanding will lead to development of advanced polymeric materials for Air Force applications. This program's approach is to study the chemistry and physics of these materials through synthesis, processing, and characterization. This area addresses both functional properties and properties pertinent to structural applications. Materials with these properties will provide capabilities for future Air Force systems to achieving global awareness, global mobility, and space operations.

Proposals with innovative material concepts that will extend our understanding of the structure-property relationship of these materials and achieve significant property improvement over current state-of-the-art materials are sought. Current interests include photonic polymers, polymers with interesting electronic properties, liquid crystals, bio-inspired materials and nanostructures.

In the area of photonic polymers, research emphases are placed on electro-optic and photorefractive polymers. Organic molecules with large multiphoton absorption cross sections are also of interest. It is desirable to increase the electro-optical coefficients of organic and polymeric materials with appropriate levels of thermal and temporal stability. Space operation issues of these polymers are also of interests. Control of speed and wavelength sensitivity in organic photorefractive polymers is currently supported. Examples of electronic properties of interest include conductivity, electrochromaticism, electroluminescence, electro-pumped lasing and superconductivity. In the area of structural properties, polymers with high thermomechanical properties are desirable. End uses of these structural polymers include aircraft and rocket components, canopies, coatings, and space structures. Issues relating to impact toughness and lifetime durability will be of special interest. Approaches based on biological systems to achieve materials properties that are difficult to achieve through conventional means are of interest. Current supports in nanostructures include controlling optical, electronic and mechanical properties and fabrication of submicron scale structures.

Material concepts that can improve on the above-mentioned optical, electronic, and mechanical properties of polymers are sought. These concepts include, but are not limited to, organic and polymeric materials, polymer blends, liquid crystals, and nanostructures.

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Surface and Interfacial Science

The objective of the Surface and Interfacial Science program is to improve the fundamental understanding of the structure and reactivity of surfaces and how they interact with their environment at the interface. This work will lead to a better understanding of the mechanisms involved in surface processes, and it will provide the foundation for the development of advanced surface structures and interfaces for future Air Force applications. The research funded under this program falls into four broad categories; surface chemistry, tribology, electrochemistry, and chemical sensing. This research investigates the basic chemical phenomena at the interface, including nucleation and growth of thin films and alloys (not to include semiconductors), friction and wear, lubrication, corrosion and materials degradation, sensing, electrochemical energy storage, and electrochemically induced reaction products and kinetics. The surface chemistry program includes efforts that are studying the mechanisms of corrosion of aluminum alloys and prevention of that corrosion. This work could potentially lead to new environmentally compliant coating systems for the protection of aging Air Force aircraft. The surface chemistry program is also funding efforts focused on the development of novel threedimensional nano-scale surface structures and systems for electronic, power, and sensing applications. Under the tribology program, research is supported into the solid, liquid, and vapor lubrication of surfaces. This work is designed to provide the Air Force with novel lubricants, lubrication systems, and wear-resistant coatings for current and future generation aircraft engines, and for micro-electromechanical (MEMS) systems in both terrestrial and space applications. The electrochemistry program has efforts investigating molten salt systems for the development of advanced materials and compact power sources for Air Force systems. Finally, work supported by this program includes chemical sensing of corrosion and wastes at the interfaces/surfaces of aircraft and their servicing environment. This may lead to development of new diagnostic tools that will alert technicians to areas of an aircraft that are experiencing corrosion, or it may provide new sensors that will help detect and monitor toxic materials and substances in the aircraft environment.

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Theoretical Chemistry

The major objective of the theoretical chemistry program is to develop new methods that can be utilized as predictive tools for designing new materials and improving processes important to the Air Force. These new methods can be applied to areas of interest to the Air Force including the structure and stability of molecular systems that can be used as advanced propellants; molecular reaction dynamics; and the structure and properties nanostructures and interfaces. Interest in advanced propellants is concentrated in the High Energy Density Matter (HEDM) Program, which aims to develop new propellant systems that can double the current payload capacity that can be put into orbit. Theoretical chemistry is used to predict promising energetic systems, to assess their stability, and to guide the efficient synthesis of selected candidates. These tools will help identify the most promising synthetic reaction pathways and predict the effects of condensed media effects on synthesis. This program is also seeking to identify novel energetic molecules and investigating the interactions that control or limit the stability of these systems. Particular interests in reaction dynamics include developing methods to seamlessly link electronic structure calculations with reaction dynamics, and using theory to describe and

predict the details of ion-molecule reactions and electron-ion dissociative recombination processes relevant to ionospheric and space effects on Air Force systems. Interest in nanostructures and materials includes work on catalysis, surface-enhanced processes mediated by plasmon resonances. This program also encourages the development of new methods and algorithms that take advantage of parallel computing architectures to predict properties with chemical accuracy for systems having a very large number of atoms that span multiple time and length scales.

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Molecular Dynamics

The objectives of the molecular dynamics program are to understand, predict, and control the reactivity and flow of energy in molecules. This knowledge will be used in atmospheric chemistry to improve our detection and control of signatures; in high-energy-density matter research to develop new energetic materials for propellants and propulsion systems; in chemical laser research to develop new high-energy laser systems; and in many other chemical systems in which predictive capabilities and control of chemical reactivity and energy flow at a detailed molecular level will be of importance.

Areas of interest in atmospheric chemistry include the dynamics of ion-molecule reactions relevant to processes in weakly ionized plasmas, atmospheric heterogeneous chemistry in aircraft and rocket exhausts, gas-surface interactions in space, and reactive and energy transfer processes that produce and affect radiant emissions in the upper atmosphere. Research on high energy density matter for propulsion applications investigates novel concepts for storing chemical energy in low-molecular-weight systems, and the stability and sensitivity of those energetic molecular systems. The coupling of chemistry and fluid dynamics in high speed reactive flows is also of interest. Research in energy transfer and energy storage in metastable states of molecules supports our interest in new concepts for chemical lasers.

Materials-related research includes the study of the synthesis, structure, and properties of metal-containing molecular clusters and nanostructures. Interest in nanostructures has particular emphasis on nanoscale systems in which the number of atoms or specific arrangement of atoms in a cluster has dramatic effects on its reactivity or properties. Also of interest are sensitive new diagnostic methods for detecting individual molecules and probing nanostructures. Fundamental studies aimed at developing basic understanding and predictive capabilities for chemical reactivity, bonding, and energy transfer processes are also encouraged.

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Chronobiology

This program supports research that provides a foundation for the development of effective measures to counter human fatigue, specifically fatigue induced by sustained wakefulness or by chronic sleep deprivation. Both circumstances are of concern to the Air Force because of

requirements for sustained operations or for shift work that is out of phase with natural biological rhythms (e.g. night operations).

Current efforts investigate the interaction of circadian and homeostatic systems in the regulation of cognitive and psychomotor performance. Human neurobehavioral data is used to develop and refine mathematical models of the circadian/homeostatic interaction. A comprehensive effort is underway to measure and integrate the various effects of behavioral routines, sleep scheduling, exposure to light, and wake-promoting pharmaceuticals.

The chronobiology program has very limited funding available for new projects. Preference is given to proposals that can contribute directly to new countermeasure developments or that open novel avenues for such developments. General investigations of circadian physiology, especially in areas supported by other federal agencies, are unlikely to be accommodated. New approaches that promise breakthroughs in understanding the cognitive and psychomotor consequences of sleep deprivation will be considered.

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Biomimetics, Biomaterials, and Biointerfacial Sciences

The goals of this biology, chemistry, and physics program are to study, use, mimic, or alter how biological systems accomplish a desired (from our point of view) task or to enable them to do a specific task in order to produce biomaterials and systems, which will enable future US Air Force technologies. This program not only wants to mimic existing biological systems, but also to create new capabilities in these organisms for more precise control over system production. The research will encompass three general areas: biomimetics, biomaterials, and biointerfacial sciences.

Biomimetic research is for enabling the development of novel sensors, engineering processes, and mechanisms. It will study the fundamental principles, processes, and designs of infrared sensitive biosystems at the sub-cellular, molecular and genomic levels to enable the further development of infrared materials, devices, and systems with enhanced structural and functional capabilities. Included are identify, model, and construct alternative biomimetic, near ambient infrared sensing devices. Finally, this program wants to probe and manipulate the functionality of alternative sensors for time-response characteristics, and adapts biochromophores and biophotoluminescent characteristics in microbial and protein-based biosystems for applications to military sensor systems.

The biomaterials area is focused on synthesis, structure, and properties of novel materials and nanostructures. Specifically, it will address either the mimicking of natural materials, using organisms as biomaterial factories of new materials, genetically altering existing organisms for new materials capabilities, or taking existing biomaterials/organisms and using them as novel materials like viral gradients or processing them further to make useful material as in biomineralization.

The biointerfacial sciences area is focused on new biosensors and bionanotechnology. Specifically, it will address the fundamental science at either the biotic-biotic or the biotic-abiotic interface. This will include both sensor arrays using combinatorial methods, and the

transduction of the desired event for display and processing. It includes most of the non-electromagnetic biosensor work as well as surface structure efforts down to the nanoscale for addressing bionanotechnology and biomesotechnology efforts.

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Cognition and Decision

This program supports research on high-order aspects of human information processing that contribute to skilled human performance. The overall objective is to describe quantitatively how humans process information to learn, recognize, assess, and make decisions about events occurring in dynamic environments. Specific objectives include, but are not limited to, the development of quantitative models and methods that improve our understanding of (a) multisensory perceptual integration, (b) cognitive and perceptual factors in the acquisition of complex skills, including motor skills, (c) team decision-making, and (d) the fundamental constraints of attention and memory on human performance. Of particular interest are models of individual and team behavior that are based on optimal rules for performing the task (such as detection or recognition, information search or integration, decision making, and resource scheduling, allocation, and coordination). A further specific objective is to improve our ability to identify and quantify the individual attributes that determine or constrain human performance, especially in complex information-processing environments. The study of these topics in conditions that involve uncertainty, high workloads, sustained operations, stress, or fatigue is encouraged. Multidisciplinary approaches are also encouraged, especially if useful in the development of quantitative or computational models of these human performance issues.

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Sensory Systems

The sensory systems program pursues an understanding of biological sensing mechanisms and investigates the integration of multiple sensory systems in human perception. Emphasis is on studies that can contribute the basic science foundation needed to inform new approaches to enhance human performance. This program supports research that coordinates empirical studies with mathematical or computational modeling. The development of theoretical models is desired, in part, for their eventual application to human factors problems, such as those that arise in the design of human systems to, for example, assist spatial orientation or navigation, find, track, and manipulate objects, or respond to acoustic information from multiple, simultaneous sources.

The current emphasis of this program is on the dynamic integration of multiple sensory inputs in human performance. One ongoing effort deals with the integration of auditory, visual, vestibular, and somatosensory inputs in response to non-standard gravito-inertial forces. Another deals with the coordination of head and eyes in tracking moving targets. A third effort studies several aspects of spatial audition, including sound localization, distance perception, and auditory cueing of visual search. The program is multi-disciplinary, drawing upon expertise in areas such as neurophysiology, computer and electrical engineering, biology, mathematics, and

experimental psychology. Applicants are encouraged to develop collaborative relationships with scientists in the Air Force Research Laboratory.

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Biological Response Profiling and Assessment

The Air Force develops and uses various physical and chemical agents that can interact with biological tissue and be potentially harmful to military and civilian personnel, to the surrounding populace, and to the environment. The agents primarily include non-ionizing radiant energies (radio frequency radiation, microwaves and laser light) and various chemicals that constitute fuels, propellants and lubricants of interest to the Air Force. Exposure to these agents may result directly from their use during Air Force operations and maintenance and, in the case of chemicals, may also occur indirectly, for example, as a result of leaky storage containers that contaminate streams, ground water, air, and soil.

To protect personnel, maintain hazard-free operational environments and develop safer materials, the Air Force supports basic research that endeavors to explore the interactions of these agents with biological systems at the cellular and molecular levels. The use of new technologies, such as transcriptomics, proteomics, and/or metabolomics, to characterize and assess the biomolecular response of cells to these agents is encouraged. Interpreting the data for mechanistic understanding and distinguishing between adverse and benign biomolecular response profiles will be especially challenging. Studies that can effectively combine novel experimental and computational techniques for the purpose of predicting toxicity will also be considered for support. Because the Air Force continually develops weapon technologies that depend on new chemicals and unique modes of radiant energies, it has become necessary to develop reliable, rapid and inexpensive methods for estimating health risks due to exposure. Mechanistically based in-vitro biomarkers combined with computational toxicology/chemistry represent research areas that may be particularly important in assessing health risks. Support of this kind of research is in harmony with an Air Force goal to minimize use of animals in research and to replace hazardous materials and processes with safe and effective alternatives. To accomplish these goals, this program promotes research that studies the interactions of biological systems with non-ionizing radiation and chemicals of unique interest to the military.

The following represent some basic research interests of the Air Force in Biological Response Profiling and Assessment:

I. CHEMICAL TOXICOLOGY

- A. Cellular/molecular mechanisms and biomarkers of toxicity
- B. Low dose, nonlinear response relationships
- C. Biomolecular response profiling
- D. In-vitro structure-activity relationships and their quantitative, computational and predictive implications
- E. Physiologically based pharmacokinetic (PBPK) modeling and metabolism of Air Force chemicals

II. LASER AND MICROWAVE RADIATION BIOEFFECTS

- A. Acute and chronic interactions of sub-nanosecond laser pulses with ocular and dermal tissues

- B. Interactions of ultra wide band and high peak power microwaves with cells/tissues
- C. Biomolecular response profiling
- D. Biomarkers of exposure and effect
- E. Biophysical and mathematical modeling of radiation-induced damage

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